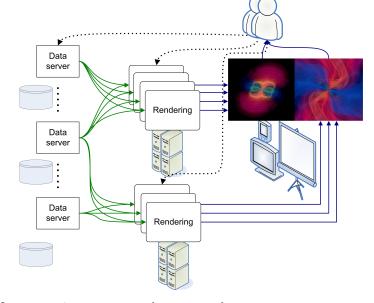


Gabrielle Allen Associate Professor Computer Science & CCT Louisiana State University



Current Area of Research Interest

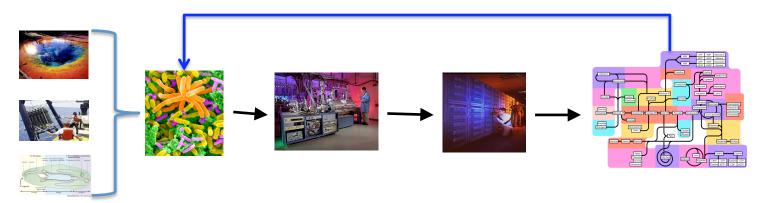
- Computational frameworks for large scale scientific applications (Cactus)
 - e.g. Petascale, debugging tools, multiphysics, web 2.0, viz, steering.
- Interactive, distributed visualization across high speed networks
- Numerical relativity, coastal modeling, CFD, advanced end-to-end scenarios

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- General strategies for coupling multi-science, multi-scale codes
- Application level tools for verification, optimization
- Modeling of relativistic astrophysics, e.g. Gamma Ray Bursts

DOE/Office of Science Opportunities in Biology at the Extreme Scale of Computing

Imaging and Computer in the Loop



Biochemical Pathways and Networks

- Application of data analysis to pathway identification
- Novel applications of proteomics and genomics
- High throughput biology as hypothesis-driven science
 - •Thousands of simultaneous hypotheses

Challenges For Advanced Computing and Mathematics

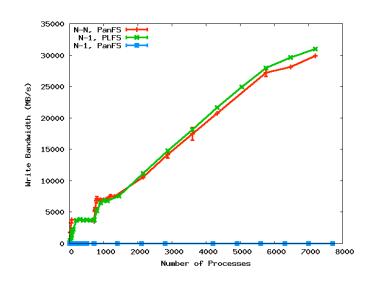
- Integration of simulation and data analysis: Scientificallyprincipled data analysis
- Structure-based modeling: Molecular simulations
 Protein folding, Enzyme mechanisms
- Social challenge: Development of HP Computational Biology applications depends on who is directing research.



Bill Cannon Senior Scientist PNNL



Garth Gibson
Professor of Computer Science
Carnegie Mellon University, and
Chief Technology Officer
Panasas Inc.



Current Area of Research Interest

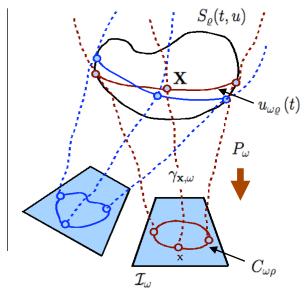
- Data storage systems at Exascale performance
- Interactive data analytics for massive science datasets

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Inferring 3D tertiary and quaternary structure of proteins from primary sequences and bio-physical data
- Understanding spatial-temporal behaviors that govern the rate of protein folding by comparative analysis of long-timescale simulations



Albert F. Lawrence Specialist IV **CRBS** University of California, San Diego



Current Area of Research Interest

- Integral Transform Theory
- Mathematical Modeling
- Tomography
- Image Processing

Challenges that May be Addressed with Advanced Computing and **Mathematics Capabilities**

- Nondestructive/Noninvasive Imaging
- Petascale Data Sets
- **Automated Reconstruction**
- Real Time Processing

High Resolution Electron Microscope Tomography for Multiscale Modeling

Problem

- Determine cellular ultrastructure over whole cells and tissues
- Obtain realistic structure for physiological modeling

Data Processing Requirements

- Scale as data acquisition rate and accuracy required from reconstruction
- Terabyte to petabyte image data sets for each cell
- Operations per full high resolution reconstruction of typical biological cell in exascale range.

Methods

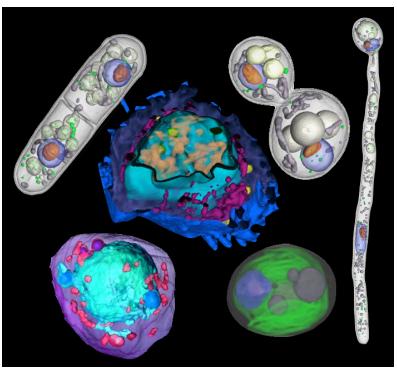
- Computer based tomography, image analysis, tracking and segmentation
- Research in transform theory, artificial intelligence, algorithms

Results

- Better understanding of life processes beyond the molecular level
- Applications to bio-engineering, bio-medicine
- Synergies with brain modeling, network theory



Name Mark Le Gros Physicist Lawrence Berkeley National Laboratory



Current Area of Research Interest

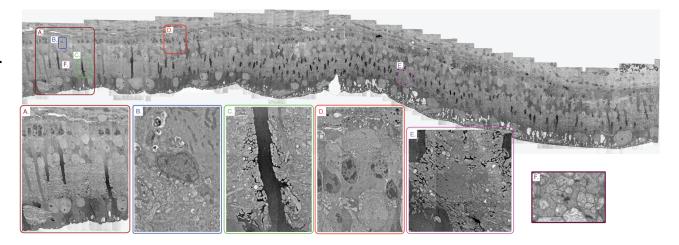
- Development of new imaging technologies, X-ray and Cryo-Light microscopy
- Multimodal studies of cell structure and function
- 3-D Whole cell imaging quantitative methods and visualization

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Data alignment and reconstruction
- Volumetric analysis of cell structure, segmentation, shape analysis
- Detailed modeling of cell structure at different stages of the cell cycle in a statistically significant cell population

Imaging and Computer in the Loop

Tolga Tasdizen
Assistant Professor
SCI Institute,
U. of Utah



Current Area of Research Interest

- Automated Neural Circuit Reconstruction
- •Volume registration and assembly from hundreds of thousands of high resolution EM images (~10 Terabytes per volume)
- Automatic annotation of volumes for neural circuit reconstruction: Segment individual neurons and find synapses.

Challenges

- Machine learning algorithms have been shown to be promising for automatic annotation, but can only be trained on small subsets or highly downsampled versions of the images. Both solutions compromise accuracy.
- •Algorithms for training can be parallelized such as batch backpropagation to take advantage of advanced computational resources.

